

Quantum computation with graphene nanoribbon

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Abstract

We propose a scalable scheme to implement quantum computation in graphene nanoribbon. It is shown that electron or hole can be naturally localized in each zigzag region for a graphene nanoribbon with a sequence of Z-shaped structure without exploiting any confined gate. An one-dimensional graphene quantum dots chain is formed in such graphene nanoribbon, where electron or hole spin can be encoded as qubits. The coupling interaction between neighboring graphene quantum dots is found to be always-on Heisenberg type. Applying the bang-bang control strategy and decoherence free subspaces encoding method, universal quantum computation is argued to be realizable with the present techniques.

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Electron spin is one of the leading candidates for the realization of a practical solid qubit [1]. The coherent manipulation of electron spins in GaAs quantum dots has been efficiently realized [2, 3]. However due to the interaction with the environment, the decoherence time is often in nanoseconds scale in GaAs quantum dots [2, 4, 5]. Even by applying the complex technique to prepare nuclear state, the dephasing time for spin qubits is just about $1\mu s$ [6]. The decoherence is one of the most challenges in the way to quantum computer in GaAs quantum dots. Due to the weak spin-orbit coupling and hyperfine interactions in carbon, graphene is argued to be an excellent candidate for quantum computation [7]. However, due to the special band structure of graphene [8], the low-energy quasiparticles in graphene behave as Dirac fermions, and the Klein tunneling and Chiral effect lead to the fact that it is non-trivial to form good quantum dot (localized electron states) in graphene. It has been shown that the massless Dirac fermions in graphene can be confined by using suitable transverse states in graphene nanoribbons (GNR) [7, 9], by combining single and bilayer regions of graphene [10, 11] or by using inhomogeneous magnetic fields [12]. Recently, there was an experiment report that GNR with well defined zigzag or armchair edge structures can be chemically produced [13]. It has also been discovered that localized states exist in the zigzag region in Z-shaped GNR [14].

Here we present a scalable quantum computation scheme based on Z-shaped GNR quantum dot system without exploiting any confined gates. The localized particle can be chosen to be electron or hole by adjusting the back gate even in the room temperature. The qubit is encoded on the electron (hole) spin states localized in the zigzag region of the GNR with a sequence of Z-shaped structure. The interaction between qubits is determined by the GNR geometrical structure and found to be Heisenberg form. By exploiting bang-bang (BB) control strategy and decoherence free subspaces (DFSs) encoding method, universal quantum gates are shown to be realizable in this system with the present techniques.

Based on the π orbital tight-binding model, the local density of state (LDOS) and the band structure of the zigzag region in a GNR with a sequence of Z-shaped structure can be obtained by the direct diagonalization of the single particle Hamiltonian $H_0 = \sum_{ij} \tau_{ij} |i\rangle \langle j|$, where the hopping matrix element $\tau_{ij} = -\tau$ if the orbits $|i\rangle$ and $|j\rangle$ are nearest neighboring on the honeycomb lattice, otherwise $\tau_{ij} = 0$ [15, 16]. From the calculated band structure, we can see that there are several localized states with electron-hole symmetry around the zero energy point as shown in Fig. 1a. Thus we can choose to get one localized electron or

hole in the zigzag region by adjusting the Fermi level through the back gate. The electron ground state energy and the energy gap between the ground state and the first excitation state are very sensitive to the size of the zigzag region, as shown in Fig 2. It has been known that the width of the armchair GNR (N unit cells) decides whether the system is metallic or semiconducting [15, 16]. If $N = 3m - 1$ (m being an integer), the armchair GNR is metallic, otherwise it is semiconducting. In addition, for the present Z-shaped structure the boundaries along the ribbon of armchair region is unsymmetrical when N is even. Actually, in our calculation we find there is no confined state in the zigzag region of Z-shaped GNR when $N = 3m - 1$ or $N = 2m$ as shown in Fig. 2. On the other hand, when N is 7 and the length of the zigzag region L (unit cells) (see Fig. 1c) is 3, 4, 5, 6, 7 and $N = 9$, $L = 3, 4$ both the ground level and energy gap are above 0.1eV. Thus we can confine electron (hole) to form quantum dot even in the room temperature.

Fig. 1b shows the spatial distribution of local density of ground state for a GNR with two Z-shaped structure in series. Each zigzag region (quantum dot) confines one electron and the quantum dots are coupled by the exchange coupling J_1 . We can obtain J_1 by calculating the exchange integral $J_1 = \int \varphi_1^*(\vec{r}_1)\varphi_2^*(\vec{r}_2)\frac{e^2}{|\vec{r}_1-\vec{r}_2|}\varphi_1(\vec{r}_2)\varphi_2(\vec{r}_1)d\vec{r}_1d\vec{r}_2$, where $\varphi_1(\vec{r})$ and $\varphi_2(\vec{r})$ are the wavefunction of neighboring graphene quantum dots. We can also calculate the next nearest neighboring exchange coupling J_2 by the same method. Obviously, the exchange coupling J_1 , J_2 are determined by the geometrical structure of the nanoribbon. For each N and L , J_1 and J_1/J_2 depend on the number of unit cells (D) between two neighboring qubits. By numerical calculations, J_1 , J_1/J_2 are obtained with different N , L , D , as shown in Fig. 3. For $N = 7$, $L = 6$, $D = 18$, $J_1 = 8\mu\text{eV}$, $J_1/J_2 = 10^5$, we can safely neglect this non-nearest neighboring qubits coupling. For clarity, in the following discussion we focus on the atomic structure with $N = 7$, $L = 6$, $D = 18$.

To carry out quantum computation, we have to form the logical qubit and realize universal quantum gate. It has been shown that single qubit rotations combined with two-qubit operations can be used to create basic quantum gates [17]. The spin of the localized electron or hole can be used as the physical qubit and the GNR with a sequence of Z-shaped structure forms an one-dimensional qubit chain as shown in Fig. 1d. The neighboring qubits in this chain have an always-on Heisenberg interaction $H = J_1\vec{S}_1 \cdot \vec{S}_2$. Here \vec{S}_1 and \vec{S}_2 are the spin operator of the neighboring localized electron (hole). It has been known that BB control strategy and DFSs encoding method do not require directly controlling the

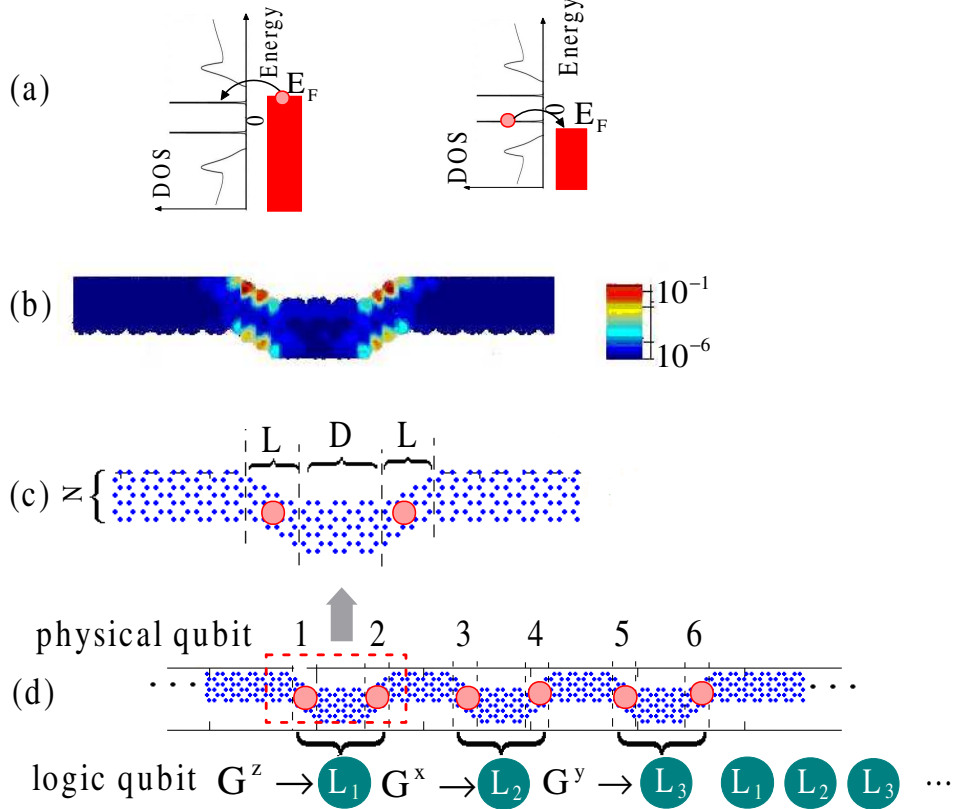


FIG. 1: (Color online) Schematic of the proposed architecture of GNR for quantum computation. (a) The Z-shaped GNR quantum dot can localize one electron (left figure) or hole (right figure) in the zigzag region by adjusting the Fermi level through the back gate. (b) Local density of states of GNR with two Z-shaped structure in series. (c) A GNR with two Z-shaped structure in series, each zigzag region confines one electron. The physical qubit is encoded into the spin of the confined electron. (d) Special encoding method to eliminate the interaction between logical qubits. Physical qubits 1 and 2 form logical qubit L_1 ; physical qubits 3 and 4 form logical qubit L_2 ; physical qubits 5 and 6 form logical qubit L_3 . The G^z , G^x , G^y are the BB operation sets of L_1 , L_2 and L_3 respectively.

interaction between qubits [18, 19]. The quantum information in qubits can be protected from decoherence induced by the environment and undesired disturbance induced by the inherent qubit-qubit interaction with these strategies.

For a sequence of Z-shaped structure GNR with $N = 7$, $L = 6$, $D = 18$, the Hamiltonian

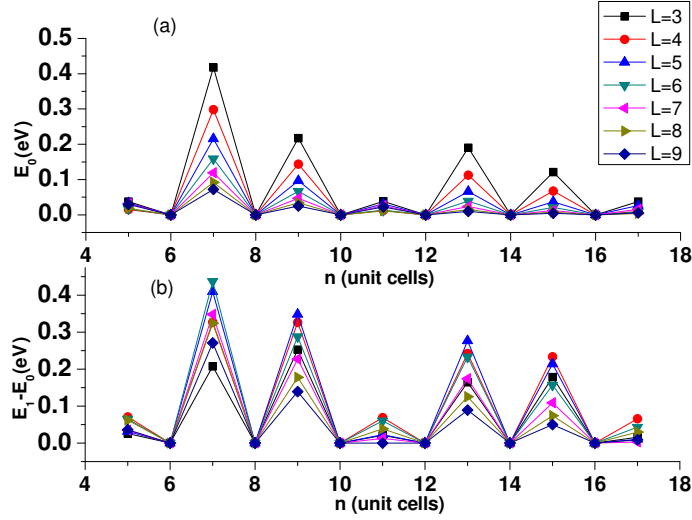


FIG. 2: (Color online) The ground energy level (E_0) and energy gap ($E_1 - E_0$) between the ground state and the first excitation state of the Z-shaped GNR quantum dot device with different width of nanoribbon (N unit cells) and different length of quantum dot region (L unit cells).

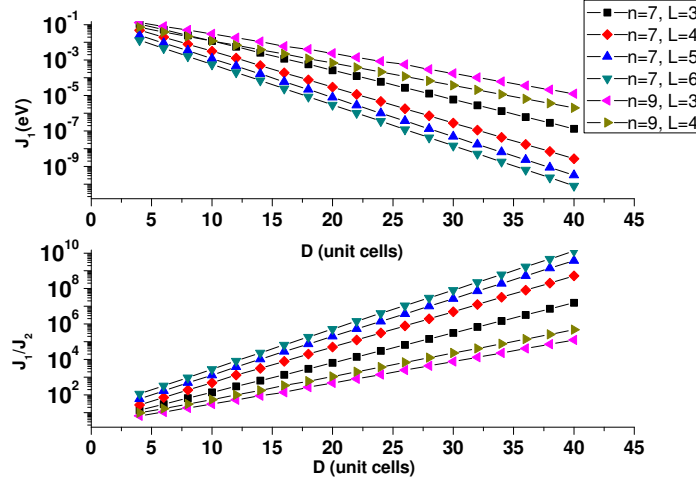


FIG. 3: (Color online) (a) The coupling energy J_1 of two nearest neighboring qubits dependence on the number of unit cells between two qubits is presented for different size of quantum dot region. (b) The ratio of J_1 to the next nearest neighboring exchange energy J_2 depend on the distance D of two neighboring qubits for different size of quantum dot region.

of the system can be expressed as

$$H_I = \sum_{i,j} J_{i,j} (\sigma_i^x \otimes \sigma_j^x + \sigma_i^y \otimes \sigma_j^y + \sigma_i^z \otimes \sigma_j^z), \quad (1)$$

where $\sigma_{i,j}^{x,y,z}$ are the spin Pauli operators of the localized electron (hole) in the quantum dots, i and j represent two neighboring dots. Here we have neglected the interaction between non-neighboring dots, which has been shown to be 5 orders smaller than the neighboring interaction.

To avoid the spin qubits to entangle with the environment, we can apply a BB operation $U_z = \exp(-i\sigma_z\pi/2)$ to each quantum dot region. Such rotation operations can be realized if a pulsed magnetic field could be applied exclusively [1]. To counteract phase decoherence, we can use DFSs encoding [20]. For a simply DFSs encoding, two physical qubits can encode a logical qubit:

$$|0\rangle_L = |\uparrow_1\downarrow_2\rangle, |1\rangle_L = |\downarrow_1\uparrow_2\rangle. \quad (2)$$

As shown in Fig. 1c, we use localized electron in the two neighboring zigzag regions to form a logical qubit.

In order to protect quantum information in the logical qubits, we must decouple the always-on Heisenberg interaction between two physical qubits within a logical qubits and interaction between two neighboring logical qubits. A nonsynchronous BB pulse operations and a special encoding method can be exploited to eliminate these interactions [19]. Here we propose an architecture in which the one-dimensional GNR chain form a periodic structure $L_1L_2L_3L_1L_2L_3 \cdots$ with three logical qubits as a unit, as shown in Fig. 1d. L_1 represents a logical qubit encoded as Eq.(2). L_2 is a logical qubit encoded as

$$|0\rangle_{L2} = \frac{1}{2}(|\uparrow\rangle_3 + |\downarrow\rangle_3)(|\uparrow\rangle_4 - |\downarrow\rangle_4), \quad (3)$$

$$|1\rangle_{L2} = \frac{1}{2}(|\uparrow\rangle_3 - |\downarrow\rangle_3)(|\uparrow\rangle_4 + |\downarrow\rangle_4). \quad (4)$$

And L_3 is a logical qubit encoded as

$$|0\rangle_{L3} = \frac{1}{2}(|\uparrow\rangle_5 + i|\downarrow\rangle_5)(|\uparrow\rangle_6 - i|\downarrow\rangle_6), \quad (5)$$

$$|1\rangle_{L3} = \frac{1}{2}(|\uparrow\rangle_5 - i|\downarrow\rangle_5)(|\uparrow\rangle_6 + i|\downarrow\rangle_6). \quad (6)$$

With this periodic architecture, we have to apply nonsynchronous BB pluse operations respectively to L_1 , L_2 , L_3 from the operation set $G^z = \{I, U_z, R_z\}$, $G^x = \{I, U_x, R_x\}$,

$G^y = \{I, U_y, R_y\}$, where $U_z = -\sigma_1^z \otimes \sigma_2^z$, $R_z = -iI_1^z \otimes \sigma_2^z$, $U_x = -\sigma_1^x \otimes \sigma_2^x$, $R_x = -iI_1 \otimes \sigma_2^x$, $U_y = -\sigma_1^y \otimes \sigma_2^y$, and $R_y = -iI_1 \otimes \sigma_2^y$. Then we obtain a quantum computation system with entirely decoupled logical qubits.

Now we show how to carry out universal quantum gates of the logical qubits defined above. Logical operations \bar{X} and \bar{Z} can generate all SU(2) transformations of logical qubit. For logical qubit L_1 , $\bar{X} = \frac{1}{2}(\sigma_1^x \otimes \sigma_2^x + \sigma_1^y \otimes \sigma_2^y)$, $\bar{Z} = \frac{1}{2}(\sigma_1^z - \sigma_2^z)$. \bar{X} can be easily achieved by recoupling qubits 1 and 2 by adjusting the BB pulses of both qubits to be synchronous [19]. The operation time can be obtained by $J\Delta t = \hbar\pi/4$, for $N = 7$, $L = 6$, $D = 18$, $\Delta t = 0.2\text{ns}$. \bar{Z} can be achieved by directly varying the Zeeman splitting on the two physical qubits individually analogous to single-qubit operations in the Loss-DiVincenzo quantum computer [1]. The operation time of this \bar{Z} gate can be about 1ns when 20mT magnetic field could be pulsed exclusively onto each quantum dot region. The fidelity of the \bar{X} gate can be effected by the fluctuation or inhomogeneity in the exchange coupling J_1 between different dots. The charge noise in the back gate can cause the fluctuation of J_1 . The main sources of the J_1 inhomogeneity between different dots are the disorder, irregular edges and defect of the GNR. Short-range disorder scarcely affects the LDOS of the ground state. The irregular edge effect and long-range disorder change the LDOS but do not destroy the confined states [14]. To get high fidelity for \bar{X} operation, we should avoid the long-range disorder and irregular edge. Actually, if we know the coupling J_1 between different dots exactly, inhomogeneity of J_1 can not effect the fidelity of \bar{X} gate when corresponding inhomogeneous operation times are used. In addition, we find the effect of the J_1 inhomogeneity or fluctuation to the fidelity of the \bar{X} gate is small as shown in Fig. 4. Because the nuclear field would change the evolution of the spin states, the fidelity of the \bar{Z} gate is dominated by the nuclear field [3]. The fidelity of the \bar{Z} gate can be very high due to small nuclear field in graphene system. Similarly, high fidelity operation \bar{X} and \bar{Z} can be also realized for logical qubits L_2 and L_3 .

We can construct CNOT gate between two neighboring logical qubits, for example L_1 and L_2 , by W gate $W = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes e^{i2\theta\bar{Z}} = e^{i\theta\bar{Z} \otimes \bar{Z}}$ and Hadamard operation [21]. By performing Hadamard transformation

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \quad (7)$$

to the two physical qubits of the second logical qubit L_2 and changing the BB control pulse to be the same with L_1 , we can recouple the two neighboring logical qubits and implement

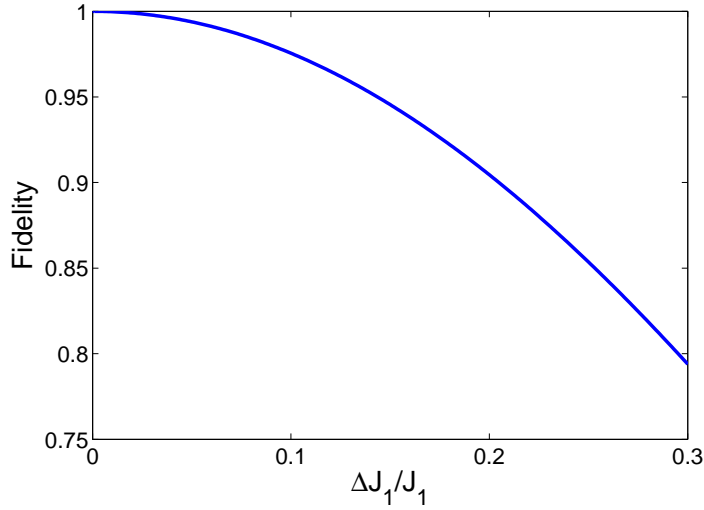


FIG. 4: The fidelity of \bar{X} gate against the fluctuation or inhomogeneity of the exchange coupling energy J_1 .

W gate of logical qubits of L_1 and L_2 . For the present graphene quantum dots chain with $N = 7$, $L = 6$, $D = 18$, the total operation time of a CNOT gate can be implemented in about 1ns with an oscillating magnetic field of 100mT to achieve the Hadamard operation. Similar to the above discussion for \bar{X} and \bar{Z} operation, we can find that the fluctuation or inhomogeneity of J_1 and the nuclear field have trivial effect to the fidelity of the CNOT gate in the present protocol.

The major decoherence sources of spin qubits in solid state system have been identified as the spin-orbit interaction and hyperfine interaction. The weak spin-orbit coupling have been predicted in carbon material due to the low atomic weight [22]. Since the primary component of natural carbon is the zero spin isotope ^{12}C , the very long coherence time given by hyperfine coupling has been theoretically argued [7]. Assuming the abundance of ^{13}C is about 1% as in the nature carbon material, the decoherence time has been predicted to be more than $10\mu\text{s}$ in the graphene quantum dot [7, 23]. This decoherence time is 4 orders longer than the gates operation time of the present protocol. In addition, the decoherence time can be much longer if the percentage of ^{13}C is decreased by isotopic purification.

In this paper we have presented a scalable scheme of quantum computation based on GNR with a sequence of Z-shaped structure. No confined gates is needed to localize the particle, which can be chosen to be electron or hole by adjusting back gate. The qubit

is encoded in electron or hole spin states, which is naturally localized in the zigzag region of GNR even in room temperature. The neighboring qubits are found to have an always-on Heisenberg interaction and the dynamical decoupling techniques with DFSs is exploited to achieve universal quantum computation in this system. Due to recent achievement in production of graphene nanoribbon, this proposal may be implementable within the present techniques.

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